A CONCEPTUAL "DESIGN" BASED METHOD FOR GENERATION OF BATCH RECIPES

I. Papaeconomou[1], S. B. Jørgensen[1], R. Gani[1] and J. Cordiner[2]
[1]CAPEC, Computer Aided Process Engineering Center,
Department of Chemical Engineering, Technical University of Denmark
DK-2800 Lyngby, Denmark

[2] Syngenta, Grangemouth Manufacturing Centre,
Earls Road Grangemouth, Stirlingshire, FK3 8XG, United Kingdom

Abstract

A simple method for generating batch recipes for a reaction and distillation operations has been developed as a part of a methodology for synthesis of batch operational sequences. The main feature of the method is that it provides near optimal solutions with respect to operational time and/or cost without using rigorous models or numerical optimization techniques. It identifies the tasks and sub-tasks that need to be performed in order to achieve a desired operational state through the shortest time/cost and without violating any operational constraints. The method also identifies the principal operational parameters and a corresponding operational model where these parameters are the main variables. The developed method is illustrated through a case study.

Keywords

Operational design, Batch recipes, Batch distillation

Introduction

A batch operation may be characterized in terms of tasks (reaction, separation, mixing or any combination of those) that need to be performed over a period of time. A batch route may be defined as a sequence of operations, performed to achieve a set of specific objectives. The synthesis of batch processes entails the identification of the necessary tasks and their sequence. However, for the synthesis to be complete, every task has to be fully characterized. Designing the operation of each batch task, where the objective is the optimization of a number of variables (time, utility costs or a weighted average of those), involves the identification of sub-tasks and the order they need to be performed in order to reach the specified objective for the overall task. The sub-tasks, for example heating, cooling, operating at a specific reflux ratio or vapour boilup rate, are defined as operations where the manipulated variables remain constant during the period of the sub-task.

The knowledge derived from the synthesis and the operational design is usually necessary before being able to plan, schedule and design control for batch operations. Existing methodologies for planning and scheduling usually do not determine the batch operational routes but use them as given data.

The majority of batch operations are frequently scaled up from the laboratory to the full size plant without much process optimization to reduce the time to markets. Our goal is to develop a conceptual design and synthesis methodology which would generate near optimum batch recipes with minimum computational effort. For the case of batch distillation, it would be useful to develop a method to identify apriori a sequence of sub-tasks that satisfy the product objectives, without using rigorous models. The algorithm developed is based on the (maximum) driving force approach, which ensures the easiest, fastest and near energy minimum operation. Determining feasible and near optimum values for the operating variables is addressed in the algorithm. A batch recipe is generated, which actually also provides the operational model needed to verify the batch

operation experimentally and/or through simulation. Dynamic simulation has been used to validate the algorithm.

Methodology

The objective for the synthesis of batch operational sequences is to minimize the operating time and/or cost of operation. The focus in some cases might be the optimal time, while in others the minimization of energy/ operating costs. As there is a trade off between these two objectives, ultimately an optimization problem will have to be formulated and solved, where appropriate weights can be given to time and operating costs.

A methodology has been developed for the synthesis of batch operational routes. This methodology consists of a set of algorithms that generate feasible/near optimum batch recipes for specified operational and end constraints. The common ground of these algorithms is the existence of a number of constraints that need to be satisfied at all time and the usage of manipulated variables to ensure feasible operation. The algorithms take care of the operational modelling of each task by identifying the sequence of sub-tasks that need to be performed in order to achieve the objectives of the specified operation. This is done with the help of a set of knowledge (thermodynamic insights) based rules, which are employed to identify the end of each sub-task and determine the next feasible sub-task.

Algorithm for batch reactor

One of the algorithms developed covers the case of batch reactors, when there is only one phase present in the system. The algorithm has been presented previously, as described by Papaeconomou et al. (2002). The problem is defined as a batch reactor where multiple reactions are taking place and operational constraints on temperature are present. Some of the reactions are desired, while others are competing reactions that need to be suppressed. There are two end objectives, namely the molefraction of the limiting reactant in the reaction of interest that should be as low as possible and the progress of the reaction of interest that should be as high as possible. At least one of the end constraints has to be satisfied. An additional constraint that is introduced in the algorithm is on selectivity.

The algorithm helps to identify the first operating step (sub-task) based on a check on selectivity. For the generation of the recipe, rules are employed at all points to identify the end of each sub-task and to determine the next feasible sub-task, such as isothermal operation, adiabatic operation, heating, cooling, etc. The procedure is repeated until the product (end) constraints are met.

Algorithm for batch distillation

The algorithm uses a set of simple equations for the distillation column and adapts well-known methods, such as the driving force approach and the McCabe-Thiele diagram to find quickly a near optimum recipe for the separation task. The batch distillation column with negligible holdup in the perforated plates and the condenser, as described in Diwekar (1995), follows also the Rayleigh equation for simple distillation. The overall material balance and the material balance for the most volatile component around the complete column result in the following equations.

$$x_D dB = d(Bx_B) = Bdx_B + x_B dB \qquad (1)$$

Integrating eqn. (1) leads to the Rayleigh equation.

$$\ln\left(\frac{B}{F}\right) = \int_{x_F}^{x_B} \frac{dx_B}{x_D - x_B} \qquad (2)$$

In the above equations, F is the initial charge, B is the amount remaining in the still, x_D is the instantaneous distillate composition and x_B is the still composition of the more volatile component.

The overall material balance around the top section:

$$dD/dt = \frac{V}{R+1} \qquad (3)$$

In the above equation, V is the vapour boilup rate, R is the reflux ratio and D is the amount of distillate.

For the batch distillation column described here the whole column is just a rectifying section. So, the functional relationship between x_D and x_B turns out to be given from the operating line equation in the enriching section of a continuous distillation column, Diwekar (1995).

$$y_j = \frac{R}{R+1} x_{j-1} + \frac{1}{R+1} x_D \qquad (4)$$

In order to identify the bottom composition x_B, the easiest method to be applied is the McCabe and Thiele graphical method. The McCabe-Thiele graphical method can be extended to batch distillation, with the assumption of equimolar overflow. In order to calculate x_B with this method, one needs to know the number of trays of the column and the reflux ratio. However, the reflux ratio cannot be chosen arbitrarily. If it is too small the separation might be infeasible. On the other hand if it is too high, the separation might be excessive energy consuming.

Therefore, it is necessary to identify the minimum reflux ratio R_{min} needed to perform the separation. One way to find R_{min} is through the driving force approach. The driving force as defined by Gani and Bek-Pedersen (2000) is the difference in composition of a component in

two co-existing phases. Thus, for the case of a batch distillation column (from eqn. (4)), it is:

$$DF = y - x = \frac{-1}{R+1}x + \frac{1}{R+1}x_D \qquad (5)$$

The existence of a driving force is what makes the distillation possible. Operating at the largest driving force leads to the near minimum energy expenses (Gani and Bek-Pedersen). From Fig. 1 it is obvious that for a specific feed composition, the largest driving force corresponds to the minimum reflux ratio. However, the minimum reflux ratio can only be supported by an infinite number of plates. Thus, for a specific number of plates a larger than the minimum reflux ratio has to be used. As the composition of the more volatile component in the still moves to the left (decreases), the reflux ratio used (R_1) approaches the minimum value for the corresponding composition ($R_{min,2}$). At that point a new reflux ratio has to be used (R_2).

The driving force gives you the physical insights to operate in an easy and near optimum energy costs way. Moreover, large driving force, which corresponds to low reflux ratio means a faster separation. This is also supported by eqn. (3), where the lowest the R, the largest the distillate rate.

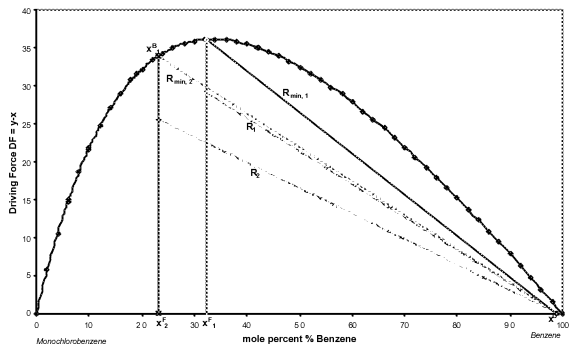

Figure 1. Driving Force diagram for the binary system Benzene-Monochlorobenzene

There are two basic modes of operation in a batch distillation column:

1. Constant reflux and variable product composition
2. Variable reflux and constant product composition of the key component

In this paper, we are considering the second mode. So, the reflux ratio is changing with time, however for a specific period it remains constant. The assumption is then made that for that period of time both the reflux ratio is constant and the distillate composition remains constant in an average value that has an allowed minimum. Taking this into account, eqn. (2) becomes:

$$B = F\frac{x_D - x_F}{x_D - x_B} \qquad (6)$$

And from the overall material balance:

$$D = F - B \qquad (7)$$

In the above equations F is the initial charge, x_F is the initial feed composition, x_D is the allowed minimum distillate composition, D is the amount distilled and B and x_B are the amount remaining in the still and its corresponding composition by the end of the period operated with a specific constant reflux ratio.

The time for that period of constant reflux ratio can be found from the integration of eqn. (3).

$$\int_0^T dt = \int_0^D \frac{R+1}{V}dD \Leftrightarrow T_{period} = \frac{R+1}{V}D \qquad (8)$$

A method is proposed in this paper to identify the sequence of periods (sub-tasks) where the column is operated at different constant reflux ratios. The algorithm developed identifies the value of the reflux ratio and the time of operation for each period.

Algorithm

The algorithm is illustrated in Fig. 2. The objective of the algorithm is to identify in advance the necessary sequence of sub-tasks in order to achieve a number of end objectives for the distillation task. These objectives are the product purity and the amount of product (yield).

The algorithm consists of a number of steps. Initially, the relationship between the vapour boilup rate and the reflux ratio has to be investigated, in order to locate operating problems, such as flooding. In that way, when the chosen reflux ratio for a sub-task is too high for the corresponding vapour boilup rate, an action can be taken.

The first sub-task (operation for period 1) is identified with the following procedure, which is then repeated until the end objectives are reached. From the known data, which are the composition of the feed and the desired product (distillate) composition, the driving force approach is employed to find the minimum reflux ratio for the specific feed.

The second step is to calculate the reflux ratio R that will match the specified number of plates of the column. This is done by a special stage by stage calculation for a distillation column using a primarily synthesis tool developed by Hostrup (2002) and implemented in ICAS (Gani et al. 1997). If the chosen reflux ratio is lower than the flooding value for the specific vapour boilup rate, the next step is to determine the bottom composition at the end of this period. Otherwise, a new value for the vapour boilup has to be selected first.

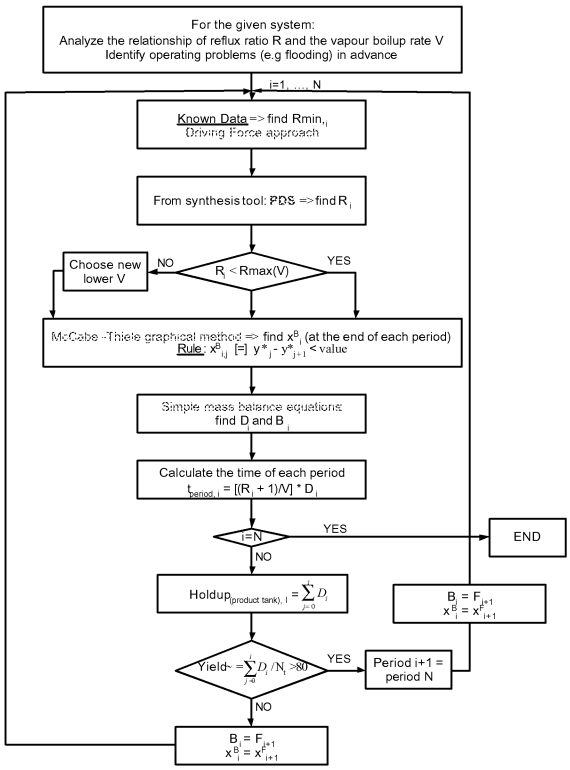

Figure 2. Schematic presentation of the algorithm for batch distillation.

The composition in the amount remaining in the still at the end of this period can be found using the simple graphical method of McCabe-Thiele. However, since the available number of plates might be excessive for the separation, the bottom composition x_B is not necessarily identified from the last plate N, but from plate j where no significant improvement in the vapour composition occurs between the adjacent plates j and j+1. The amount D distilled in this period and the amount B remaining in the still, as well as the operating time (end) of this sub-task are calculated (from eqns (6), (7) and (8). The next step, in effect, is the designation of the bottom composition x_B and the amount in the bottom B as the feed composition x_F and the feed F for the next sub-task.

Repeating the above described procedure directs to the synthesis of a batch recipe for a batch distillation column. The last sub-task is identified as the one where the yield of the product achieved in the previous sub-task is above a high value of 80 percent.

A case study

A problem given in Perry's Handbook, 7th ed. (example 13-10) was considered. The algorithm was applied for the ternary system of benzene, monochlorobenzene (MCB) and o-dichlorobenzene (DCB). The objective was a 99% purity benzene with a 95% yield. Benzene and MCB was considered as a binary system. The algorithm provided the batch recipe, which consisted of six sub-tasks.

Table 1. Batch recipe for obtaining benzene

Period no	Reflux ratio	Vapour boilup rate	Period time, hr
1	1.264	100	0.0919
2	1.969	100	0.0441
3	2.65	100	0.0597
4	3.865	100	0.0618
5	6.654	80	0.0993
6	11.962	80	0.0954

The simulation engine in ICAS (Gani et al. 1997) for batch processes, BRIC, has been employed for dynamic simulation to verify the suggested recipe. The only additional constraint for the rigorous simulation was on the distillate composition, which was not allowed to drop below the purity objective, except on the last sub-task where it was not taken into account. Both the product objectives were reached (product purity=99% and yield=97.3%>95%). Compared to operation with a constant reflux ratio, where both product objectives are achieved, the time and the generated recipe is by 40% faster and energy efficient.

Conclusions

A simple algorithm that can handle the operational modelling of multicomponent batch distillation has been developed. The algorithm without using any rigorous models can generate apriori a batch recipe that satisfies the product objectives. The algorithm has been tested for obtaining the first product of a ternary system. The validation with rigorous simulation proved successful. The recipe was also superior to constant reflux operation

Acknowledgements

We are grateful to Syngenta and Joan Cordiner for supporting this research.

References

Diwekar, U.M. (1995). *Batch Distillation. Simulation, Optimal Design and Control*. Taylor & Francis, USA.

Gani, R., Hytoft, G., Jaksland, C. and Jensen, A.K. (1997). *Comp. & Chem. Eng.*, **21**, 1135-1146.

Gani, R. and Bek-Pedersen, E. (2000). *AIChE J.* **46** (6), 1271-1274.

Hostrup, M. (2002). *Integrated Approach to Computer Aided Process Synthesis.* Ph.D.-thesis. DTU, Denmark.

Papaeconomou, I., Gani, R., Jørgensen, S.B. (2002). A General Framework for the Synthesis and Operational Design of Batch Processes. *Comput. Chem. Eng., (In Press).*